

Band gaps induced by vacuum photons in closed semiconductor cavities

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We consider theoretically a closed (zero-dimensional) semiconductor microcavity where confined vacuum photonic mode is coupled to electrons in valence band of the semiconductor. It is shown that vacuum-induced virtual electron transitions between valence and conduction bands result in renormalization of electron energy spectrum. As a consequence, vacuum-induced band gaps appear within the valence band. Calculated values of the band gaps are of sub-meV scale, that makes this QED effect to be measurable in state-of-the-art experiments.

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Introduction.— There are physical situations where the electron-photon interaction cannot be considered as a weak perturbation (so-called regime of strong light-matter coupling). In this regime, it is necessary to consider the system “electron + field” as a whole. Such a bound electron-photon object, which was called “electron dressed by field” (dressed electron), became commonly used model in modern physics [1, 2]. The interest in this field is stimulated by the possibility of the achievement of the hybrid — half-light half-matter — excitations which can demonstrate peculiar properties. Therefore, the regime of strong light-matter coupling was extensively investigated both theoretically and experimentally in a variety of the systems, including optical planar microcavities with semiconductor [3–5] and organic [6–8] quantum wells, microcavities with individual quantum dots [9–11] and others. Effects of strong coupling can be used for variety of technological applications [12], including novel types of the lasers [13, 14], optical switches and logic gates [15–17], all-optical integrated circuits [18], sources of entangled photon pairs [19] and others. Among most bright phenomena of strong light-matter coupling, we have to note the field-induced modification of energy spectrum of dressed electrons — also known as a dynamic (ac) Stark effect — which was discovered in atoms many years ago [20] and has been studied in details in various atomic and molecular systems [1, 2]. For solids, the dynamic Stark effect results in the gap opening within electron energy bands [21–25].

In order to turn usual “bare” electrons into “dressed” electrons, a characteristic energy of electron-photon interaction should be increased. This can be done in two different ways. The first of them consists in using a strong laser-generated electromagnetic field (the case of large photon occupation numbers) [1, 2]. The second way consists in decreasing the effective volume where electron-

photon interaction takes place. This can be realized with embedding an electron system inside a microcavity [12, 26]. It should be stressed that there is no formal physical difference between “real” photons (quanta of electromagnetic wave) and “virtual” ones (quanta of vacuum fluctuations inside a cavity). Therefore, the strong coupling of electrons to vacuum photonic mode inside a cavity can open energy gaps in various solids in the same way as an usual dynamic Stark effect. To study this phenomenon, the new area of interdisciplinary theoretical research at the border between quantum electrodynamics and physics of semiconductors was opened during last years. In the previous papers on the subject [27–29], the vacuum-induced modification of electron energy spectrum in solids was studied exclusively for *opened* cavities, including both two-dimensional cavities and one-dimensional ones. Unfortunately, vacuum-induced gaps in these cavities are very small. As a consequence, experimental observation of the gaps is very difficult since the scattering of conduction electrons in real solids washes the gaps. Therefore, it is necessary to find physical objects where the discussed effects can be observable in state-of-the-art experiments. In the given Brief Report, we will demonstrate that the vacuum-induced gaps can be giant in *closed* (zero-dimensional) cavities of macroscopically large size.

Model. — Let us consider a semiconductor embedded inside a closed (zero-dimensional) cavity [see Fig. 1(a)]. In what follows, we will assume that the cavity dimensions (L_x, L_y, L_z) are macroscopically large as compared with characteristic de-Broglie wave length of the electrons. Therefore, the electron energy spectrum of conduction and valence bands of the considered semiconductor sample are the same as for bulk semiconductor, $\varepsilon_{v,c}(\mathbf{k}) = \pm \varepsilon_g/2 \pm \hbar^2 k^2/2m_{v,c}$, where ε_g is the semiconductor band gap, $m_{v,c}$ are the electron effective masses in valence and conduction bands, \mathbf{k} is the electron wave vector. Interacting with vacuum photonic mode of the cavity, valence electrons perform virtual transitions between valence and conduction bands [see Fig.1(b)], which

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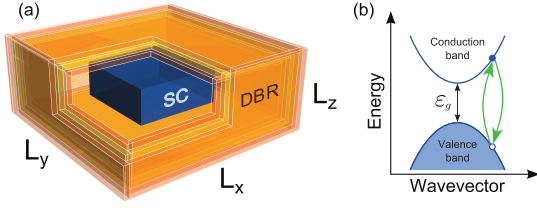


FIG. 1. (Color online) (a) Sketch of the system under consideration: a bulk semiconductor (SC) embedded into a closed (zero-dimensional) microcavity formed by distributed Bragg reflectors (DBR) with dimensions (L_x, L_y, L_z); (b) Electron energy spectrum of the bulk semiconductor with vacuum-induced (virtual) interband electron transitions marked by the arrows.

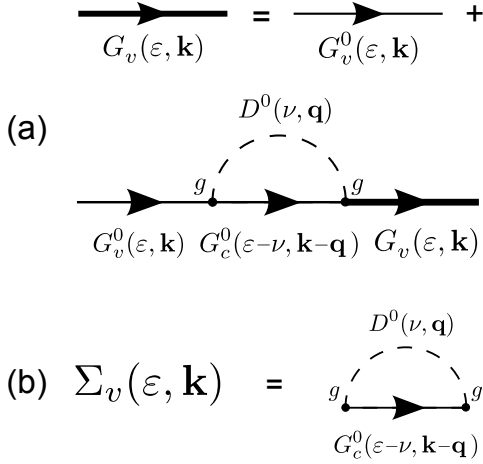


FIG. 2. (a) The Dyson equation for renormalized electron Green's functions corresponding to the valence band; (b) The self-energy operator responsible for the photon-induced dressing of the valence band. The dashed line corresponds to a virtual cavity photon and g denotes the electron-photon coupling constant.

modify the electron energy spectrum. In order to find the renormalized spectrum of valence electrons, ε , let us apply the conventional diagrammatic approach based on Green's functions.

Generally, a dressed electron in the valence band with the energy ε and the wave vector \mathbf{k} is described by the Dyson equation [see Fig. 2(a)] which can be written in the algebraic form as

$$G_v(\varepsilon, \mathbf{k}) = \frac{G_v^0(\varepsilon, \mathbf{k})}{1 - \Sigma_v(\varepsilon, \mathbf{k})G_v^0(\varepsilon, \mathbf{k})}, \quad (1)$$

where the self-energy for valence electrons interacting with cavity photons [see Fig. 2(b)] is defined by the expression

$$i\Sigma_v(\varepsilon, \mathbf{k}) = \sum_{\mathbf{k}'} g^2(\mathbf{k}', \mathbf{k}) \int \frac{d\nu}{2\pi} iD^0(\nu) iG_c^0(\varepsilon - \nu, \mathbf{k}'), \quad (2)$$

$G_c^0(\varepsilon, \mathbf{k}) = (\varepsilon - \varepsilon_c(\mathbf{k}) - i0)^{-1}$ is the Green's function for bare conduction electron, $G_v^0(\varepsilon, \mathbf{k}) = (\varepsilon - \varepsilon_v(\mathbf{k}) + i0)^{-1}$

is the Green's function for bare valence electron,

$$D^0(\nu) = \frac{2\omega}{(\nu - \omega + i0)(\nu + \omega - i0)} \quad (3)$$

is the photon Green's function, ν is the photon energy, ω is the eigenenergy of cavity photons, and $g(\mathbf{k}', \mathbf{k})$ is the electron-photon coupling constant. The sought dispersion relation of valence electrons dressed by vacuum fluctuations, $\varepsilon(\mathbf{k})$, is given by the poles of the renormalized Green function (1). These poles are defined by the equation

$$1 - \Sigma_v(\varepsilon, \mathbf{k})G_v^0(\varepsilon, \mathbf{k}) = 0. \quad (4)$$

As to the electron-photon coupling constant, within the dipole approximation it can be written as

$$g(\mathbf{k}', \mathbf{k}) = \left| \langle \psi_c(\mathbf{k}'), 0 | \hat{\mathbf{d}} \hat{\mathbf{E}} | \psi_v(\mathbf{k}), 1 \rangle \right|, \quad (5)$$

where $\psi_{v,c}(\mathbf{k})$ are electron wave functions in the valence and conduction bands, the symbols (0, 1) describes the photon occupation numbers of the cavity mode, $\hat{\mathbf{d}}$ is the operator of electric dipole moment,

$$\hat{\mathbf{E}} = i\sqrt{\frac{\omega}{2\varepsilon\epsilon_0}} [\hat{a}^\dagger \mathbf{u}^* - \hat{a} \mathbf{u}] \quad (6)$$

is the operator of electric field corresponding to the cavity photon eigenmode \mathbf{u} , and \hat{a} , \hat{a}^\dagger are the operators of annihilation and creation of photons in the cavity eigenmode. In order to simplify the calculations, let us restrict our consideration to the case of $L_z \ll L_{x,y}$. Then eigenmodes of the cavity photons are described by the expression

$$\mathbf{u}(\mathbf{r}) \approx \mathbf{e} \sqrt{\frac{8}{V}} \sin(q_z z) \sin(q_x x) \sin(q_y y), \quad (7)$$

where $\mathbf{r} = (x, y, z)$ is the radius-vector written in the Cartesian coordinates, $V = L_x L_y L_z$ is the cavity volume, $\mathbf{e} = (e_x, e_y)$ is the polarization vector of the cavity eigenmode, $q_{x,y,z} = \pi l_{x,y,z} / L_{x,y,z}$ are characteristic photon wave vectors of the eigenmode, and $l_{x,y,z} = \pm 1, \pm 2, \pm 3, \dots$. Then, taking into account the electron interaction with a ground photon mode of the cavity, we can write eigenenergy of cavity photons as $\omega \approx \hbar c \pi / L_z$. Substituting Eqs. (6)–(7) into the Eq. (5), we get

$$g^2(\mathbf{k}', \mathbf{k}) = \frac{|d_{cv}|^2}{16} \frac{\omega}{\varepsilon\epsilon_0 V} \sum_{\mathbf{q}} \delta_{\mathbf{k}', \mathbf{k}-\mathbf{q}} \quad (8)$$

where the photon wave vector of ground eigenmode is

$$\mathbf{q} = \left(\frac{\pi n_x}{L_x}, \frac{\pi n_y}{L_y}, \frac{\pi n_z}{L_z} \right), \quad (9)$$

$n_{x,y,z} = \pm 1$, and d_{cv} is the interband matrix element of the dipole moment at $\mathbf{k} = 0$. Within the Kane model of semiconductor band structure [35], this matrix element can be written as $|d_{cv}| \approx |\hbar| / \sqrt{2m_c \varepsilon_g}$.

Results and discussion. — In order to find the energy spectrum of dressed valence electrons, ε , we have to solve Eq. (4). This equation can be solved analytically in the approximation of negligibly small photon wave vector ($q \approx 0$), when the coupling constant (8) takes the simple form

$$g^2(\mathbf{k}', \mathbf{k}) \approx \frac{\omega |d_{cv}|^2}{2\epsilon\epsilon_0 V} \delta_{\mathbf{k}', \mathbf{k}}. \quad (10)$$

Substituting the constant (10) into Eq. (2), we arrive at the self-energy

$$\begin{aligned} \Sigma_v(\varepsilon, \mathbf{k}) &= i \frac{\omega |d_{cv}|^2}{2\epsilon\epsilon_0 V} \\ &\times \int \frac{d\nu}{2\pi} \frac{2\omega}{(\nu - \omega + i0)(\nu + \omega - i0)(\varepsilon - \nu - \varepsilon_c(\mathbf{k}) - i0)}. \end{aligned} \quad (11)$$

Performing contour integration in Eq. (11) over the upper half-plane, $\text{Im}(\nu) > 0$, and applying the residue theorem, we can write the self-energy (11) as

$$\Sigma_v(\varepsilon, \mathbf{k}) = \frac{\omega |d_{cv}|^2}{2\epsilon\epsilon_0 V [\varepsilon + \omega - \varepsilon_c(\mathbf{k})]}. \quad (12)$$

Then Eq. (4) is

$$[\varepsilon + \omega - \varepsilon_c(\mathbf{k})][\varepsilon - \varepsilon_v(\mathbf{k})] - \frac{\omega d_{cv}^2}{2\epsilon\epsilon_0 V} = 0 \quad (13)$$

and immediately gives the sought energy spectrum of the valence band modified by vacuum fluctuations,

$$\begin{aligned} \varepsilon &= \frac{\varepsilon_c(\mathbf{k}) + \varepsilon_v(\mathbf{k})}{2} - \frac{\omega}{2} \\ &- \frac{\eta(\mathbf{k})}{2} \sqrt{[\omega - \varepsilon_c(\mathbf{k}) + \varepsilon_v(\mathbf{k})]^2 + 4(\hbar\Omega_R)^2}, \end{aligned} \quad (14)$$

where $\Omega_R = |d_{cv}| \sqrt{\omega/2\epsilon\epsilon_0 V \hbar^2}$ is the effective Rabi frequency of the considered electron-photon system, and

$$\eta(\mathbf{k}) = \begin{cases} -1, & \omega > [\varepsilon_c(\mathbf{k}) - \varepsilon_v(\mathbf{k})] \\ 1, & \omega < [\varepsilon_c(\mathbf{k}) - \varepsilon_v(\mathbf{k})] \end{cases}.$$

It follows from Eq. (14) that vacuum fluctuations induce the energy gap

$$\Delta\varepsilon = 2\hbar\Omega_R = |d_{cv}| \sqrt{\frac{2\omega}{\epsilon\epsilon_0 V}} \quad (15)$$

within the valence band at electron wave vectors, \mathbf{k} , satisfying the resonant condition $\omega = [\varepsilon_c(\mathbf{k}) - \varepsilon_v(\mathbf{k})]$.

The gapped energy spectrum (14) is pictured schematically in Fig. 3(a). Outside the approximation of $q \approx 0$, we have to solve Eq. (4) numerically with using exact expression for the coupling constant (8). Due to finite value of the photonic wavevector \mathbf{q} , the vacuum-induced gap acquires fine structure: Instead of a single gap, several gaps appear [see Fig. 3(b)]. Positions of the gaps

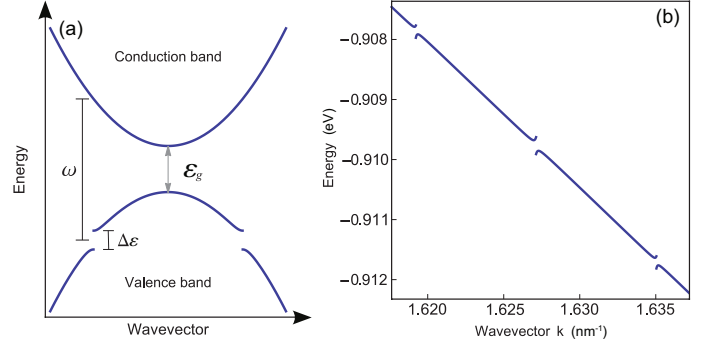


FIG. 3. (Color online) (a) Energy spectrum of dressed electrons within the approximation of a negligible small photon wavevector; (b) Exact energy spectrum of dressed valence electrons, calculated numerically for GaAs microcavity with dimensions $L_z = 100$ nm and $L_x = L_y = 500$ nm for the electron wave vector $\mathbf{k} = (k_x, k_y, k_z)$ with the components $k_x = k_y = k/\sqrt{2}$ and $k_z = 0$.

TABLE I. Vacuum-induced band gaps, $\Delta\varepsilon$, calculated for various semiconductor cavities with dimensions $L_x = L_y = 5L_z$.

Semiconductor	CdTe	ZnO	GaN	GaAs
L_z (nm)	100	85	88	100
$\Delta\varepsilon$ (meV)	0.36	0.28	0.27	0.38

in the \mathbf{k} space are defined by the resonant condition, $\varepsilon_c(\mathbf{k} - \mathbf{q}) - \varepsilon_v(\mathbf{k}) = \omega$, where the photon wave vector of the cavity eigenmode, \mathbf{q} , is given by Eq. (9).

In Tab. I, we present values of vacuum-induced band gaps which are calculated for various semiconductors using Eq. (15). It is seen that the gaps are around meV and, therefore, are several orders of magnitude larger compared to the vacuum corrections of energies of individual atoms in the absence of the cavity (for instance, the Lamb shift). It should be noted also that the calculated values of the gap for closed (zero-dimensional) cavities, given in Tab. I, essentially exceed values of the vacuum-induced gaps appearing in open (two-dimensional and one-dimensional) cavities [27–29]. Physically, the increasing of gap values in closed (zero-dimensional) cavities as compared with open ones arises from the strong (delta-function-like) singularity in the density of photon states. In order to observe the photon-induced gaps experimentally, angle-resolved photoemission spectroscopy (ARPS) looks to be most appropriate. Indeed, ultraviolet laser-based ARPS [30, 31] provides sub-meV resolution which is enough for detecting gap values given in Tab. I. As to dissipation processes arisen from nonideal structure of the cavity, they lead to the finite spectral linewidth of the cavity mode, Γ (see, e.g., Refs. [32–34]). Correspondingly, the photon-induced gaps, $\Delta\varepsilon$, are observable under the condition of $\Delta\varepsilon > \Gamma$. This condition can be easily satisfied for the gaps given in Tab. I since modern technologies allow to fabricate microcavities with

the spectral linewidth $\Gamma \sim 10^{-5}$ eV [33]. It should be noted also that closed cavities of very high quality allow to detect the vacuum Rabi splitting in individual quantum dots, which is less than the gaps given in Tab. I [34]. As a consequence, the predicted effect can be observed in state-of-the-art experiments.

Conclusion. — We calculated energy spectrum of valence electrons in closed (zero-dimensional) semiconductor cavities, which is modified by vacuum fluctuations of electromagnetic field. The feature of the spectrum consists in vacuum-induced energy gaps of sub-meV scale

within valence band, which can be observed experimentally. As a consequence, the discussed effect can open new area of interdisciplinary experimental research where quantum electrodynamics and physics of solids meet.

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